Heat capacity of Schottky type in low-dimensional spin system

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The heat capacity of low-dimensional spin systems is studied using theoretical and numerical techniques. Keeping only two energy states, the system is mapped onto the two -level-system (TLS) model. Using the low temperature Lanczos method, it is confirmed that the behavior of T_M and the energy gap as functions of the control parameter is the same in the two models studied; a conclusion that can probably be extrapolated to the general case of any system that possesses an energy gap.

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I. INTRODUCTION

Gaps in the energy spectrum play a crucial role in condensed matter physics. Fundamental properties in superconductivity or in the fractional quantum Hall effect originate from the existence of a gap between the ground state and the excited states. In particular, low dimensional quantum spin systems are extremely interesting to study the behavior of the gap. Many exact and numerical results on the one dimensional quantum spin systems with nearest neighbor couplings have been accumulated during last decades.

The 1D spin-1/2 system has been solved by Bethe[1] in 1931 with his famous ansatz. The ansatz allows the computation of the energy eigenvalues. The isotropic 1D spin-1/2 system with nearest neighbor couplings is gapless. The anisotropic spin-1/2 chain is denoted by the XXZ model[2,3]. The Hamiltonian of the XXZ model on a periodic chain of N sites is

$$H = J\sum_{i=1}^{N} S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z, \qquad (1)$$

where $J > 0$ is the exchange coupling in the xy easy plane, Δ is the anisotropy in the z direction. The Ising regime is governed by $\Delta > 1$ and there is a gap in the excitation spectrum, while for $\Delta \leq -1$, the ground state is in the ferromagnetic phase and there is a gap over the ferromagnetic state. In the region $-1 < \Delta \leq 1$, the ground state of the system, is in the gapless spin-fluid phase.

The spin-1 system is not solvable with the Bethe ansatz or similar techniques. The anisotropic spin-1 chain is only gapless[4] in the region $-1 < \Delta < 0$. Haldane[5] formulated in 1983 his famous conjecture that quantum spin chains (isotropic) with integer spin $S = 1, 2, ..$ have a gap, where as chains with half-integer spin $S = 1/2, 3/2, ...$ are gapless.

During the last two decades ladder-systems[6] as quantum spin systems between one and two dimensions have been studied as well with numerical methods. Concerning the ground state properties has been found that, ladder-systems with an even number of legs ($l = 2, 4, 6, ...$) have a gap; those with an odd number ($l = 1, 3, 5, ...$) do not. In particular, since the antiferromagnetic two-leg ladder systems have a gap in the spin excitation spectrum, they reveal extremely rich quantum behavior in the presence of a magnetic field[7]. Such quantum phase transitions in spin systems with gapped excitation spectrum were indeed studied experimentally[8,9,10,11,12,13].

On the other hand, investigating the behavior of the energy gap of spin systems in vicinity of quantum critical points has attracted much interest recently[3,14,15,16]. In general, the critical point of an thermodynamic system in the Hamiltonian formulation is defined as the value at which the energy gap vanishes as a power low, which is known as the scaling behavior. The opening of the energy gap in the vicinity of the quantum critical point is found to scale with a critical exponent. The value of the critical gap exponent is very important to find the universality class of a continuous quantum phase transition.

The discovery of gapless or gaped excitations have led to the investigation of the thermodynamic properties. One of the most important thermodynamic functions is the heat capacity. Usually, there is a lambda-type anomaly in figure of the heat capacity versus temperature. It was interpreted as indicating a phase transition to a magnetically ordered phase. An important characteristic of the low-dimensional magnets is the absence of the long range order in models with a continuous symmetry at any finite temperature[17]. There is also a broad maximum in the plot of the heat capacity vs temperature, characteristic of low dimensional systems. This is known as the Schottky peak.

In this paper, theoretical and numerical results are reported for the low-temperature behavior of the heat capacity in low dimensional spin systems. Theoretically, by keeping only two lowest states, the system is mapped to the well known two-level-system (TLS) model. In this case, the heat capacity is found exactly as a function of the energy gap and the temperature. It is shown that the position of the Schottky heat capacity peak, T_M, and the energy gap behaves in the same way as a function of the control parameter. In Section II, the mapping to the TLS model is explained and the theoretical results are

presented. In Section III, the results of the low temperature Lanczos calculations are presented. Numerically, T_M as a function of the control parameter is computed for "the alternating spin-1/2 chains in a magnetic field h" and "the 1D Heisenberg Hamiltonian with a staggered magnetic field h_s". Finally, the summary and conclusions are presented in Section IV

II. LOW TEMPERATURE LIMIT HEAT CAPACITY: TWO LEVEL SYSTEM APPROACH

In this section we discuss a theoretical approach to find the effect of the energy gap on the heat capacity of the quantum spin systems. Spectrum energy of a quantum system may be gapful or gapless. Since, we are going to study the sign of the gap on the heat capacity, gapful systems are considered. At very low temperature we can consider only lowest energy levels. If we keep only two lowest energy states, the system maps to the two level system (TLS) model[18]. We have assumed that the energy gap of this TLS is g where $E_1 = E_0 + g$, E_0 and E_1 are the ground and first exited states respectively.

Our purpose is to determine the behavior of the heat capacity for the quantum spin systems. The heat capacity is expressed by the following relation

$$C_v = \frac{1}{K_B T^2}\left[\frac{\partial^2 \ln Z}{\partial \beta^2}\right]. \tag{2}$$

where Z is the partition function denoted by

$$Z \;=\; \mathrm{Tr}\left\{e^{-\beta H}\right\}, \tag{3}$$

Here $\beta = \frac{1}{K_B T}$, K_B is the Boltzmann constant and T is temperature. We have assumed that $K_B = 1$. At very low temperature limit (TLS limit), we can write

$$Z \simeq e^{-\beta E_0} + e^{-\beta E_1} = e^{-\beta E_0}(1 + e^{-\beta g}), \tag{4}$$

And finally from the above equation one can shows

$$C_v = \frac{x^2}{\cosh^2(x)}, \tag{5}$$

where we defined $x = \frac{g}{2T}$. This result predict a Schottky like peak of the heat capacity behavior versus the x variation. The position of the Schottky peak takes place at $x_M \simeq 1.2$, where we have: $\tanh(x_M) = 1/x_M$. This result shows explicitly an upward increase of the heat capacity versus the magnetic field for $x < x_M$ and monotonic decrease for $x > x_M$. We have plotted the thermal behavior of Eq. 5 in Fig. 1. Here, x_M corresponds to the position of the Schottky peak, T_M, in a constant gap value. It is clear that by increasing the gap value, $|g|$, the peak approach to higher temperature and inversely. Therefore we can conclude that width of the energy gap may affect the position of the Schottky heat capacity peak. At very low temperature regime, all gapped thermodynamic systems ($N \to \infty$, $N =$ number of the spins) can be mapped to the above TLS model.

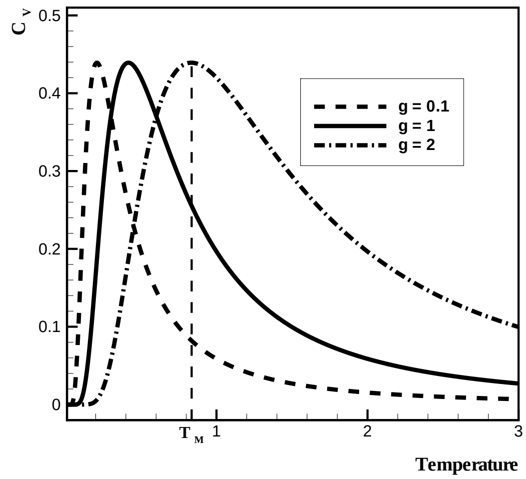


FIG. 1: Temperature dependence of the heat capacity of TLS (Eq. 5) for different energy gap values (g). T_M shows the position of the Schottky heat capacity peak for the system with $g = 2$.

Up to now we did not consider any degeneracy. In the general case both first two energy levels (TLS) have a degeneracy. It is well known for two level system (TLS) that the account of degeneracy leads to change the effective gap and consequently to change the T_M for Schottky anomaly of heat capacity[19]. In peresent of degeneracy by a little of manipulation, one can shows

$$C_v = \frac{x^2}{\cosh^2(x + x')}, \tag{6}$$

which is very similar to Eq. 5. Here we denoted $x' = \frac{g_s}{2T}$, and $g_s = T \ln \frac{d_2}{d_1}$. Where d_1 and d_2 have been considered for the order of the degeneracy of the ground state and first exited state of the system respectively. As we mentioned it before this result predict a Schottky like peak in the heat capacity behavior. The Schottky heat capacity peak takes place at x_M which satisfied $\tanh(x_M + x'_M) = 1/x_M$, where $x'_M = \frac{g_s}{2T_M}$. If we assumed that $d_1 < d_2$ then $g_s < 0$ and therefore the generalized gap $(g+g_s)$ will be smaller than the gap. Thus the Schottky peak moves to the higher values of the gap in respect to the case $g_s = 0$ (without degeneracy). In same manner for the case: $d_2 < d_1$ we have $g_s > 0$, therefore the generalized gap will be larger than the gap. Thus the Schottky peak moves to the lowest values of the gap in respect to the case $g_s = 0$.

III. NUMERICAL RESULTS

In recent years, numerical methods have been extensively developed and applied to quantum many-body problems. Most frequently used numerical method for

these problems is the exact diagonalization of small systems employing the Lanczos technique[20]. The exact diagonalization of small correlated systems does not have any restrictions on the model. The deficiency of the method is in the relative smallness of system sizes. So far the method has been essentially restricted to the evaluation of the $T = 0$ static and dynamical quantities, i.e., properties of the ground state.

Jaklič et.al. introduced a method for the evaluation of finite-temperature properties, based on the Lanczos diagonalization technique for small systems[21]. This method, is avoid the calculation of all eigenfunctions of the system. Instead, they introduced the procedure where the sampling over all states is reduced to a random partial sampling, while only approximate ground state and excited state wave functions, generated by the Lanczos technique, are used for the evaluation of matrix elements. The size limitations of the method are effectively comparable to those encountered in the Lanczos-type diagonalization technique applied to the ground state calculations.

In following, we present our numerical results on the heat capacity of the several 1D spin-1/2 models which are obtained by the method of Jaklič.

A. Alternating Heisenberg Spin-1/2 Chains in a Transverse Magnetic Field

In this section we consider the alternating spin-1/2 chains in a magnetic field. Since, the antiferromagnetic-ferromagnetic (AF-F) chains have a gap in the spin excitation spectrum, they reveal extremely rich quantum behavior in the presence of the magnetic field.

The ground state phase diagram of the AF-F alternating chain in a magnetic field is studied by the numerical diagonalization and the finite-size scaling based on the conformal field theory[22]. It is shown that the magnetic state is gapless and described by the Luttinger liquid phase. It is also found that the magnetic state is characterized by the algebraic decay of the spin correlation functions. Recently, Yamamoto et.al described the magnetic properties of the model in a magnetic field in terms of the spinless fermions and the spin waves[23]. They employed the Jordan-Wigner transformation and treated the fermionic Hamiltonian within the Hartree-Fock approximation. They have also implemented the modified spin wave theory to calculate the thermodynamic functions as the heat capacity and the magnetic susceptibility. More recently, using numerical Lanczos method, the effect of an uniform transverse magnetic field on the ground state phase diagram of a spin-1/2 AF-F chain with anisotropic ferromagnetic coupling is studied[24]. The Hamiltonian of the model under consideration on a periodic chain of N sites is given by

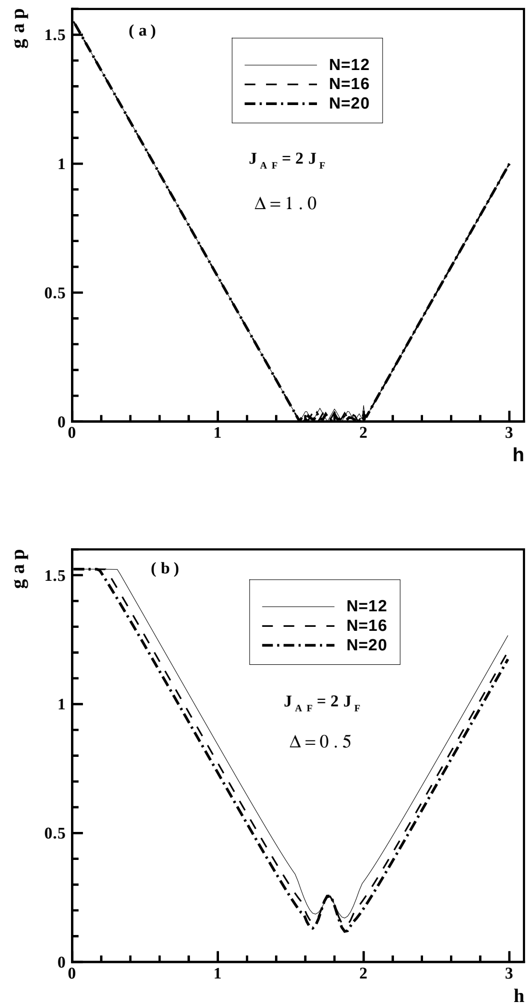


FIG. 2: a. The excitation gap of a spin-1/2 AF-F chain for isotropic case $\Delta = 1.0$ in the uniform magnetic field for different size number ($N = 12, 16, 20$). b. The excitation gap of a spin-1/2 AF-F chain in the uniform transverse magnetic field with anisotropic ferromagnetic coupling $\Delta = 0.5$, for different size number ($N = 12, 16, 20$).

$$
\begin{aligned}
H &= J_{AF} \sum_{j=1}^{N/2} [S^x_{2j-1} S^x_{2j} + S^y_{2j-1} S^y_{2j} + S^z_{2j-1} S^z_{2j}] \\
&- J_F \sum_{j=1}^{N/2} [S^x_{2j} S^x_{2j+1} + S^y_{2j} S^y_{2j+1} + \Delta S^z_{2j} S^z_{2j+1}] \\
&+ h \sum_{j=1}^{N} S^x_j . \qquad (7)
\end{aligned}
$$

Where $S^{x,y,z}_j$ are spin-1/2 operators on the j-th site. J_F and J_{AF} denote the ferromagnetic and antiferromagnetic couplings respectively. The limiting case of

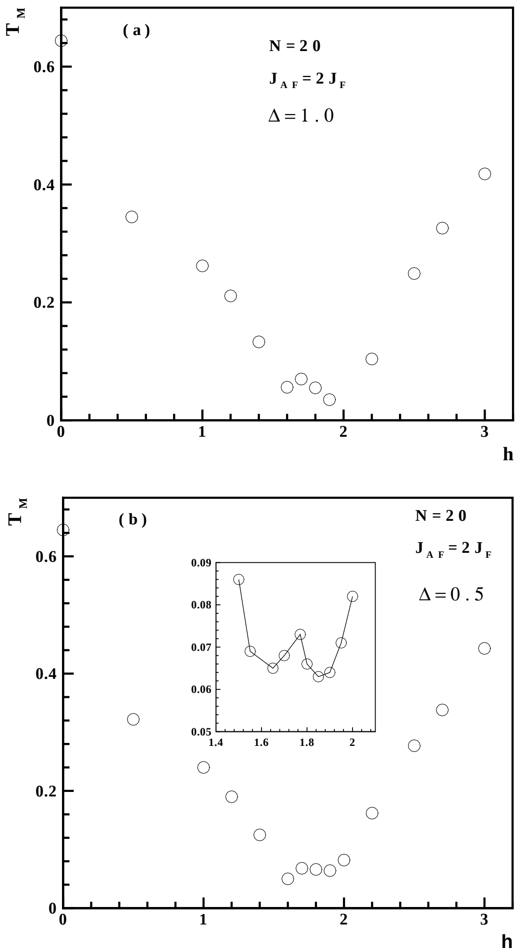


FIG. 3: a. The Schottky heat capacity peak value, T_M, versus the transverse magnetic field, for a spin-1/2 AF-F chain, and isotropic case $\Delta = 1.0$ in the uniform transverse magnetic field for system size: $N = 20$. b. The Schottky heat capacity peak value, T_M, as a function of the magnetic field, for a spin-1/2 AF-F chain in the uniform transverse magnetic field with anisotropic ferromagnetic coupling: $\Delta = 0.5$, and size number: $N = 20$. The inset shows the same quantity in the intermediate magnetic field region, $h_{c_1} < h < h_{c_2}$.

isotropic ferromagnetic coupling corresponds to $\Delta = 1$ and h is the transverse magnetic field. To explore the nature of the excitation spectrum, we use the modified Lanczos method to diagonalize numerically finite chains ($N = 12, 16, 20, 24$). The energies of the few lowest eigenstates were obtained for the chains with periodic boundary conditions. First, we have computed the three lowest energy eigenvalues of $N = 12, 16, 20$ chain with $J_{AF} = 2J_F$ and different values of the anisotropy parameter Δ.

In Fig. 2a we have plotted results of calculations for the isotropic case $\Delta = 1.0$. The excitation gap is determined[24] in the system as the difference between the first excited state and the ground state. As it is clearly seen from this figure in the case of zero magnetic field the spectrum of the model is gapped. For $h \neq 0$ the gap decreases linearly with h and vanishes at the critical field, $h_{c_1} = 1.55 \pm 0.01$. This is the first level crossing between the ground state energy and the first excited state. To get an accurate estimate of h_{c_1} we have obtained the first level crossing for system sizes of $N = 12, 14, ..., 24$. The finite size behavior of these values lead us to $h_{c_1} = 1.55 \pm 0.01$ for $N \longrightarrow \infty$. The spectrum remains gapless for $h_{c_1} < h < h_{c_2}$ and becomes once again gapped for $h > h_{c_2} = 2.0$. With increasing field, for $h > h_{c_2}$ the gap increases linearly with h. In the region $h_{c_1} < h < h_{c_2}$ we also observe numerous additional level crossing between the lowest eigenstates. These level crossing lead to incommensurate effects that manifest themselves in the oscillatory behavior of the spin correlation functions. All crossings disappear at $h > h_{c_2}$ and the correlation functions do not contain oscillatory terms in this region of the phase diagram.

In marked contrast with the isotropic case, the similar analysis of the few lowest levels for an anisotropic AF-F chain in the presence of a transverse magnetic field reveal a principally different behavior. The gap as a function of the transverse magnetic field h has been computed for the anisotropy parameter $\Delta = 0.5$ and different chain lengths $N = 12, 16, 20$. In Fig.2b we have plotted results of these calculations. As it is seen from the figure, the excitation spectrum in this case is gapful except at the two critical fields $h_{c_1} = 1.64 \pm 0.01$ and $h_{c_2} = 1.88 \pm 0.01$[24]. We have employed the phenomenological renormalization group (PRG) method[25] to determine these critical fields (h_{c_1} and h_{c_2}). The PRG equation is

$$(N + 4)gap(N + 4, h') = Ngap(N, h), \tag{8}$$

where $gap(N, h) = E_1(N, h) - E_0(N, h)$ is the energy gap value for chain length N in a magnetic field h. At the critical point, $N(E_1 - E_0)$ should be size independent for large enough systems in which the contribution from irrelevant operators is negligible. Thus, we accurately determined the critical points by the PRG method. We defined $h_c(N, N + 4)$ as the N-dependent fixed point of Eq. 8, and it is extrapolated to the thermodynamic limit in order to estimate h_c. At the critical point $h = h' = h_c$, therefore, the curves of $N(E_1 - E_0)$ vs h for sizes N and $N + 4$ cross at certain values $h_{c_1}(N, N + 4)$ and $h_{c_2}(N, N + 4)$ (finite-size critical points). The thermodynamic critical points (h_{c_1} and h_{c_2}) are obtained by appropriately extrapolating $h_{c_1}(N, N+4)$ or $h_{c_2}(N, N+4)$ to $N \to \infty$.

In the region $h_{c_1} < h < h_{c_2}$ the spin gap, which appears at $h > h_{c_1}$, first increases vs external field and after passing a maximum decreases to vanish at h_{c_2}. At $h > h_{c_2}$ the gap once again opens and, for a sufficiently large transverse field becomes proportional to h. To study the finite-temperature properties of the model, we have used the Jaklič formalism. We have computed a hundred lowest eigenvalues of the energies. We have considered different values of the transverse magnetic field,

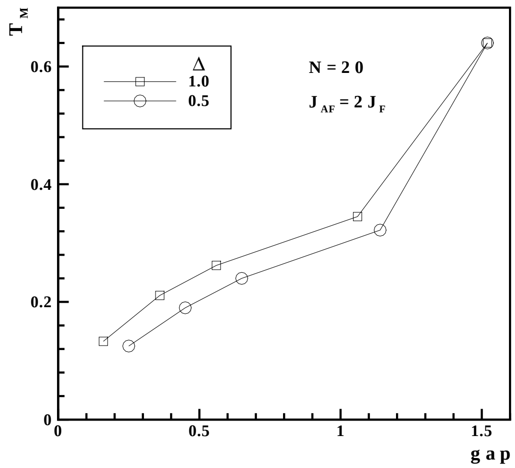


FIG. 4: The Schottky heat capacity peak value, T_M, versus the energy gap for a spin-1/2 AF-F chain with anisotropic ferromagnetic couplings: $\Delta = 1.0$ and $\Delta = 0.5$, and size number: $N = 20$.

h, and anisotropy parameter Δ. Therefore using these hundred eigen-energies, we have computed the heat capacity as a function of the temperature (T). The position of the Schottky heat capacity peak, T_M is determined as T_M. In Fig. 3a we have plotted T_M as a function of the magnetic field h. To arrive at this plot, we have considered $J_{AF} = 2J_F$, $\Delta = 1$ and $N = 20$. As it is clearly seen from this figure, the position of the Schottky heat capacity peak, T_M, T_M, decreases by increasing the magnetic field up to the critical field, h_{c_1}. In the intermediate region of the magnetic filed, $h_{c_1} < h < h_{c_2}$, T_M is independent of magnetic field. The anomaly behavior is the result of the finite size effects. With increasing the magnetic field, for $h > h_{c_2}$, T_M increases almost linearly.

It is surprising which the behavior of T_M versus the magnetic field is in complete agreement with the gap behavior respect to the magnetic filed. Thus we conclude that the energy gap sign on the position of the Schottky heat capacity peak. To confirm our idea, we have plotted T_M vs the transverse magnetic field for $J_{AF} = 2J_F$, the anisotropy parameter $\Delta = 0.5$ and $N = 20$ in Fig. 3b. As we can see from this figure for low transverse magnetic field, $h < h_{c_1}$, the behavior of T_M is the same as the isotropic case. But in the intermediate region, $h_{c_1} < h < h_{c_2}$, T_M first increases vs transverse field and after passing a maximum, decreases up to h_{c_2} (see the inset of the Fig. 3b). For the higher transverse magnetic field, $h > h_{c_2}$, the position of the Schottky heat capacity peak increases as a previous one. This behavior of the T_M is in complete agreement with the effect of the transverse magnetic field on the energy gap (Fig. 2b).

Finally, we have plotted T_M versus the energy gap for $N = 20$, $J_{AF} = 2J_F$ and different values of the anisotropy parameter $\Delta = 0.5, 1.0$. For convenience, the numerical results of the region $h < h_{c_1}$ are showed. It is clearly seen, that the possition of the Schottky heat capacity peak T_M, increases by increasing the energy gap of the system. This is in well agreement with results obtained within the two-level model.

B. The 1D AF-Heisenberg model in a staggered field

The general feature developed for the alternating spin-1/2 chains in a magnetic field can be applied to the 1D Heisenberg Hamiltonian with a staggered magnetic field h_s,

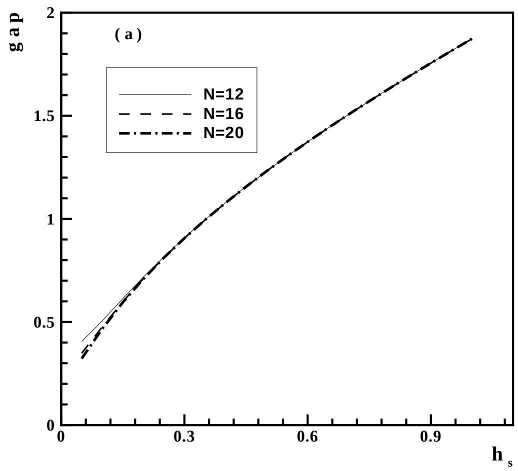
$$H = J \sum_{i=1}^{N} [\overrightarrow{S}_i . \overrightarrow{S}_{i+1} + h_s (-1)^i S_i^z]. \tag{9}$$

It is expected[26,27,28,29] that the staggered field induces an excitation gap in the $S = \frac{1}{2}$ AF-Heisenberg chain, which should be otherwise gapless. The excitation gap caused by the staggered field is indeed found in the real magnets[30,31,32]. In the absence of the staggered field ($h_s = 0$), the eigenspectra is exactly solvable. In the case of the staggered magnetic field ($h_s \neq 0$), the integrability is lost. The staggered magnetic field produces an antiferromagnetic ordered (Neel order) ground-state.

To examine the effect of the staggered magnetic field on the energy gap, we have implemented the modified Lanczos algorithm for finite-size chains $N = 12, 16, 20$ using periodic boundary conditions. The energy gap is determined as the difference between the first excited state and the ground state[14], and calculated for different chain lengths and staggered fields h_s. The energy gap is determined as the difference between the first excited state and the ground state[14].

We have plotted, in Fig. 5a, the energy gap versus the staggered magnetic field h_s. The results have been plotted for different chain sizes $N = 12, 16, 20$. It can be seen, that the spectrum is gapless in the absence of the staggered magnetic field ($h_s = 0$). The application of a staggered magnetic field, induces a gap in the spectrum of the model. With increasing the field, for $h_s > 0$, the energy gap increases with h_s.

Applying the Jakliĉ method we have computed a hundred lowest energies for different values of the staggered magnetic field. The heat capacity is computed as a function of the temperature. In Fig. 5b, the position of the Schottky anomaly heat capacity peak, T_M is plotted versus h_s for the chain size $N = 20$. As it is seen from the figure, T_M in this case increases by increasing the staggered magnetic field. This result is in good agreement with the idea that the gap sign on the position of the Schottky heat capacity peak, T_M.



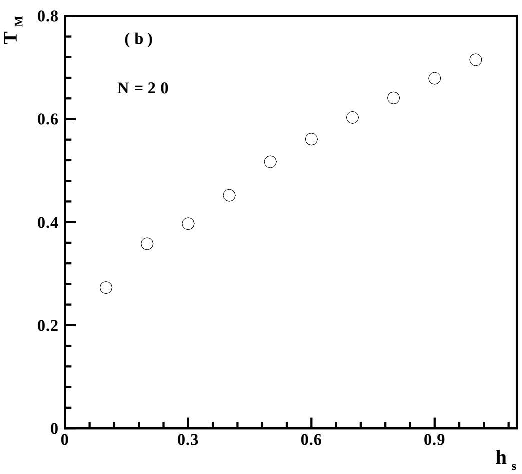


FIG. 5: a. The excitation gap of the 1D AF-Heisenberg model in a staggered field as a function of the magnetic field for different size number ($N = 12, 16, 20$). b. The position of the Schottky heat capacity peak, T_M, for the 1D AF-Heisenberg model in a staggered field versus the staggered magnetic field with size number: $N = 20$.

IV. SUMMARY AND DISCUSSION

Low temperature behavior of the heat capacity of the low-dimensional spin systems is studied using theoretical and numerical approaches. Theoretically, the system is mapped to the well known two-level-system (TLS) model. In this case, the heat capacity is found exactly as a function of the energy gap and the temperature. The position of the Schottky heat capacity peak, T_M, is determined. It is shown that T_M as a function of the control parameter behaves in the same way as the energy gap versus the control parameter. This shows that the gap has an influence on the position of the Schottky heat capacity peak.

Numerically, the finite temperature Lanczos method is applied. The Lanczos method is implemented to obtain a hundred of lowest excited state energies. This formalism is applied to two model chains up to $N = 24$ in length. First, the alternating spin-1/2 chains in a magnetic field are considered. Since, the antiferromagnetic-ferromagnetic (AF-F) chains have a gap in the spin excitation spectrum, they reveal extremely rich quantum behavior in the presence of the magnetic field. The energy gap and heat capacity are computed for both isotropic and anisotropic cases. The numerical results are computed for different values of the external magnetic field. It is shown, in complete agreement with the theoretical results, the field-dependence of the T_M and the energy gap are the same. Finally, the 1D Heisenberg model with a staggered magnetic field h_s is investigated. It is shown that the staggered field induces an excitation gap in the $S = \frac{1}{2}$ AF-Heisenberg chain, which should be otherwise gapless. Using the above numerical procedure, the position of the Schottky heat capacity peak is computed. It is confirm, that the energy gap sign on the Schottky heat capacity peak.

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[1] H. A. Bethe Zphys. **77**, 205 (1931); *ibid*,**150**, 327, (1966).
[2] Kurmann J, Thomas H, and Müller G, Physica **A 112**, 235 (1966); *ibid*,**150**, 327, (1966).
[3] D. V. Dmitriev, V. Ya. Krivnov, and A. A. Ovchinnikov, Phys. Rev. **B 65**, 172409 (2002); D. V. Dmitriev, V. Ya. Krivnov, A. A. Ovchinnikov and A. Langari, JETP, **95**, 538 (2002).
[4] Wei Chen, Kazuo Hida, and B. C. Sanctury, Phys. Rev. B **67**, 104401 (2003).
[5] F. D. M. Haldane, Phys. Rev. Lett. **50**, 1153 (1983).
[6] E. Dogotto and T. M. Rice, Sci. **271**, 618 (1996).
[7] K. P. Schmidt and G. S. Uhrig, Mod. Phys. Lett. b **19**, 1179 (2005).
[8] G. Chaboussant, P. A. Crowell, L. P. Levy, O. Piovesana,

A. Madouri and D. Mailly, Phys. Rev. B **55**, 3046 (1997).
[9] G. Chaboussant, M-H. Julien, Y. Fagot-Revurat, M. Hanson, L. P. Levy, C. Berthier, M. Horvatic and O. Piovesana, Euro. Phys. J. B **6**, 167 (1998).
[10] G. Chaboussant, Y. Fagot-Revurat, M-H. Julien, M. Hanson, C. Berthier, M. Horvatic, L. P. Levy, and O. Piovesana, Phys. Rev. Lett. **80**, 2713 (1998).
[11] D. Arcon, A. Lappas, S. Margadonna, K. Prassides, E. Ribera, J. Veciana, C. Rovira, R. T. Henriques, and M. Almeida, Phys. Rev. B **60**, 4191 (1999).
[12] H. Myaffre, H. Horvatic, C. Berthier, M-H. Julien, P. Söransan, L. P. Levy, and O. Piovesana, Phys. Rev. Lett. **85**, 4795 (2000).
[13] B. C. Watson, V. N. Kotov, N. W. Meisel, D. W. Hall, G. E. Granroth, W. T. Montfrooij, S. E. Nagler, D. A. Jensen, R. Backov, M. A. Petruska, G. E. Fanucci, and D. R. Talham, Phys. Rev. Lett. **86**, 5168 (2001).
[14] S. Mahdavifar, Euro. Phys. J. B **55**, 371, (2007).
[15] S. Mahdavifar, Euro. Phys. J. B **59**, 285, (2007).
[16] S. Mahdavifar, J. Phys: Condens. Matter.19, 406222 (2007).
[17] N. D. Mermin, H. Wagner, Phys. Rev. Lett. **17**, 1133, (1966).
[18] For example see: R. Cubo, Statistical Mechanics, Mir, Moscow, (1967).
[19] For example see: B.Wunderlich, H.Baur, Adv. Polymer Sci.**7**,151 Heat capacity of linear high polymers, (1970)
[20] C. Lanczos, J. Res. Natl. Bur. Stand. **45**, 255, (1950).
[21] J. Jaklič and P. Prelovšec, Phys. Rev. B **7**, 5065, (1994).
[22] T. Sakai: J. Phys. Soc. Jpn. **64**, 251 (1995).
[23] S. Yamamoto et. al,: Fiz. Nizk. Temp. **31**, 974 (2005).
[24] S. Mahdavifar, and A. Akbari, Accepted to J. Phys. Soc. Jpn (2007).
[25] M. N. Barber: *Phase Transitions and Critical Phenomena* , edited by C. Domb and J. L. Lebowitz (Academic Press, New York, 1983) vol. **8**, 146.
[26] M. Oshikawa and I. Affleck, Phys. Rev. Lett. **79**, 2883 (1997); Phys. Rev. B **60**, 1038 (1999).
[27] Y. -J. Wang, F. H. L. Essler, M. Fabrizio and A. A. Nersesyan, Phys. Rev. B **66**, 024412 (2002).
[28] M. Sato and M. Oshikawa, Phys. Rev. B **69**, 054406 (2004)
[29] F. C. Alcaraz and A. L. Malvazzi, J. Phys. A **28**, 1521 (1995).
[30] D. C. Dender, P. R. Hammar, D. H. Reich, C. Broholm and G. Aeppli, Phys. Rev. Lett. **79**, 1750 (1997).
[31] M. Kohgi, K. Iwasa, J. M. Mignot, B. Fak, P. Gegenwart, M. Lang, A. Ochiai, H. Aoki and T. Suzuki, Phys. Rev. Lett. **86**, 2439 (2001).
[32] R. Feyerherm, S. Abens, D. Gunther, T. Ishida, M. Meibner, M. Meschke, N. Nogami and M. Steiner, J. Phys. Condens. Matter **12**, 8495 (2000).

Heat capacity of Schottky type in low-dimensional spin system

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The heat capacity of low-dimensional spin systems is studied using theoretical and numerical techniques. Keeping only two energy states, the system is mapped onto the two -level-system (TLS) model. Using the low temperature Lanczos method, it is confirmed that the behavior of T_M and the energy gap as functions of the control parameter is the same in the two models studied; a conclusion that can probably be extrapolated to the general case of any system that possesses an energy gap.

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I. INTRODUCTION

Gaps in the energy spectrum play a crucial role in condensed matter physics. Fundamental properties in superconductivity or in the fractional quantum Hall effect originate from the existence of a gap between the ground state and the excited states. In particular, low dimensional quantum spin systems are extremely interesting to study the behavior of the gap. Many exact and numerical results on the one dimensional quantum spin systems with nearest neighbor couplings have been accumulated during last decades.

The 1D spin-1/2 system has been solved by Bethe[1] in 1931 with his famous ansatz. The ansatz allows the computation of the energy eigenvalues. The isotropic 1D spin-1/2 system with nearest neighbor couplings is gapless. The anisotropic spin-1/2 chain is denoted by the XXZ model[2,3]. The Hamiltonian of the XXZ model on a periodic chain of N sites is

$$H = J\sum_{i=1}^{N} S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z, \qquad (1)$$

where $J > 0$ is the exchange coupling in the xy easy plane, Δ is the anisotropy in the z direction. The Ising regime is governed by $\Delta > 1$ and there is a gap in the excitation spectrum, while for $\Delta \leq -1$, the ground state is in the ferromagnetic phase and there is a gap over the ferromagnetic state. In the region $-1 < \Delta \leq 1$, the ground state of the system, is in the gapless spin-fluid phase.

The spin-1 system is not solvable with the Bethe ansatz or similar techniques. The anisotropic spin-1 chain is only gapless[4] in the region $-1 < \Delta < 0$. Haldane[5] formulated in 1983 his famous conjecture that quantum spin chains (isotropic) with integer spin $S = 1, 2, ..$ have a gap, where as chains with half-integer spin $S = 1/2, 3/2, ...$ are gapless.

During the last two decades ladder-systems[6] as quantum spin systems between one and two dimensions have been studied as well with numerical methods. Concerning the ground state properties has been found that, ladder-systems with an even number of legs ($l = 2, 4, 6, ...$) have a gap; those with an odd number ($l = 1, 3, 5, ...$) do not. In particular, since the antiferromagnetic two-leg ladder systems have a gap in the spin excitation spectrum, they reveal extremely rich quantum behavior in the presence of a magnetic field[7]. Such quantum phase transitions in spin systems with gapped excitation spectrum were indeed studied experimentally[8,9,10,11,12,13].

On the other hand, investigating the behavior of the energy gap of spin systems in vicinity of quantum critical points has attracted much interest recently[3,14,15,16]. In general, the critical point of an thermodynamic system in the Hamiltonian formulation is defined as the value at which the energy gap vanishes as a power low, which is known as the scaling behavior. The opening of the energy gap in the vicinity of the quantum critical point is found to scale with a critical exponent. The value of the critical gap exponent is very important to find the universality class of a continuous quantum phase transition.

The discovery of gapless or gaped excitations have led to the investigation of the thermodynamic properties. One of the most important thermodynamic functions is the heat capacity. Usually, there is a lambda-type anomaly in figure of the heat capacity versus temperature. It was interpreted as indicating a phase transition to a magnetically ordered phase. An important characteristic of the low-dimensional magnets is the absence of the long range order in models with a continuous symmetry at any finite temperature[17]. There is also a broad maximum in the plot of the heat capacity vs temperature, characteristic of low dimensional systems. This is known as the Schottky peak.

In this paper, theoretical and numerical results are reported for the low-temperature behavior of the heat capacity in low dimensional spin systems. Theoretically, by keeping only two lowest states, the system is mapped to the well known two-level-system (TLS) model. In this case, the heat capacity is found exactly as a function of the energy gap and the temperature. It is shown that the position of the Schottky heat capacity peak, T_M, and the energy gap behaves in the same way as a function of the control parameter. In Section II, the mapping to the TLS model is explained and the theoretical results are

presented. In Section III, the results of the low temperature Lanczos calculations are presented. Numerically, T_M as a function of the control parameter is computed for "the alternating spin-1/2 chains in a magnetic field h" and "the 1D Heisenberg Hamiltonian with a staggered magnetic field h_s". Finally, the summary and conclusions are presented in Section IV

II. LOW TEMPERATURE LIMIT HEAT CAPACITY: TWO LEVEL SYSTEM APPROACH

In this section we discuss a theoretical approach to find the effect of the energy gap on the heat capacity of the quantum spin systems. Spectrum energy of a quantum system may be gapful or gapless. Since, we are going to study the sign of the gap on the heat capacity, gapful systems are considered. At very low temperature we can consider only lowest energy levels. If we keep only two lowest energy states, the system maps to the two level system (TLS) model[18]. We have assumed that the energy gap of this TLS is g where $E_1 = E_0 + g$, E_0 and E_1 are the ground and first exited states respectively.

Our purpose is to determine the behavior of the heat capacity for the quantum spin systems. The heat capacity is expressed by the following relation

$$C_v = \frac{1}{K_B T^2}\left[\frac{\partial^2 \ln Z}{\partial \beta^2}\right]. \tag{2}$$

where Z is the partition function denoted by

$$Z \; = \; \mathrm{Tr}\left\{e^{-\beta H}\right\}, \tag{3}$$

Here $\beta = \frac{1}{K_B T}$, K_B is the Boltzmann constant and T is temperature. We have assumed that $K_B = 1$. At very low temperature limit (TLS limit), we can write

$$Z \simeq e^{-\beta E_0} + e^{-\beta E_1} = e^{-\beta E_0}(1 + e^{-\beta g}), \tag{4}$$

And finally from the above equation one can shows

$$C_v = \frac{x^2}{\cosh^2(x)}, \tag{5}$$

where we defined $x = \frac{g}{2T}$. This result predict a Schottky like peak of the heat capacity behavior versus the x variation. The position of the Schottky peak takes place at $x_M \simeq 1.2$, where we have: $\tanh(x_M) = 1/x_M$. This result shows explicitly an upward increase of the heat capacity versus the magnetic field for $x < x_M$ and monotonic decrease for $x > x_M$. We have plotted the thermal behavior of Eq. 5 in Fig. 1. Here, x_M corresponds to the position of the Schottky peak, T_M, in a constant gap value. It is clear that by increasing the gap value, $|g|$, the peak approach to higher temperature and inversely. Therefore we can conclude that width of the energy gap may affect the position of the Schottky heat capacity peak. At very low temperature regime, all gapped thermodynamic systems ($N \to \infty$, $N =$ number of the spins) can be mapped to the above TLS model.

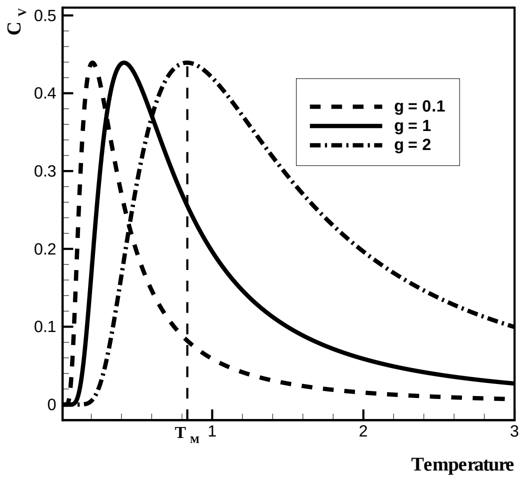

FIG. 1: Temperature dependence of the heat capacity of TLS (Eq. 5) for different energy gap values (g). T_M shows the position of the Schottky heat capacity peak for the system with $g = 2$.

Up to now we did not consider any degeneracy. In the general case both first two energy levels (TLS) have a degeneracy. It is well known for two level system (TLS) that the account of degeneracy leads to change the effective gap and consequently to change the T_M for Schottky anomaly of heat capacity[19]. In peresent of degeneracy by a little of manipulation, one can shows

$$C_v = \frac{x^2}{\cosh^2(x + x')}, \tag{6}$$

which is very similar to Eq. 5. Here we denoted $x' = \frac{g_s}{2T}$, and $g_s = T \ln \frac{d_2}{d_1}$. Where d_1 and d_2 have been considered for the order of the degeneracy of the ground state and first exited state of the system respectively. As we mentioned it before this result predict a Schottky like peak in the heat capacity behavior. The Schottky heat capacity peak takes place at x_M which satisfied $\tanh(x_M + x'_M) = 1/x_M$, where $x'_M = \frac{g_s}{2T_M}$. If we assumed that $d_1 < d_2$ then $g_s < 0$ and therefore the generalized gap $(g + g_s)$ will be smaller than the gap. Thus the Schottky peak moves to the higher values of the gap in respect to the case $g_s = 0$ (without degeneracy). In same manner for the case: $d_2 < d_1$ we have $g_s > 0$, therefore the generalized gap will be larger than the gap. Thus the Schottky peak moves to the lowest values of the gap in respect to the case $g_s = 0$.

III. NUMERICAL RESULTS

In recent years, numerical methods have been extensively developed and applied to quantum many-body problems. Most frequently used numerical method for

these problems is the exact diagonalization of small systems employing the Lanczos technique[20]. The exact diagonalization of small correlated systems does not have any restrictions on the model. The deficiency of the method is in the relative smallness of system sizes. So far the method has been essentially restricted to the evaluation of the $T = 0$ static and dynamical quantities, i.e., properties of the ground state.

Jaklič et.al. introduced a method for the evaluation of finite-temperature properties, based on the Lanczos diagonalization technique for small systems[21]. This method, is avoid the calculation of all eigenfunctions of the system. Instead, they introduced the procedure where the sampling over all states is reduced to a random partial sampling, while only approximate ground state and excited state wave functions, generated by the Lanczos technique, are used for the evaluation of matrix elements. The size limitations of the method are effectively comparable to those encountered in the Lanczos-type diagonalization technique applied to the ground state calculations.

In following, we present our numerical results on the heat capacity of the several 1D spin-1/2 models which are obtained by the method of Jaklič.

A. Alternating Heisenberg Spin-1/2 Chains in a Transverse Magnetic Field

In this section we consider the alternating spin-1/2 chains in a magnetic field. Since, the antiferromagnetic-ferromagnetic (AF-F) chains have a gap in the spin excitation spectrum, they reveal extremely rich quantum behavior in the presence of the magnetic field.

The ground state phase diagram of the AF-F alternating chain in a magnetic field is studied by the numerical diagonalization and the finite-size scaling based on the conformal field theory[22]. It is shown that the magnetic state is gapless and described by the Luttinger liquid phase. It is also found that the magnetic state is characterized by the algebraic decay of the spin correlation functions. Recently, Yamamoto et.al described the magnetic properties of the model in a magnetic field in terms of the spinless fermions and the spin waves[23]. They employed the Jordan-Wigner transformation and treated the fermionic Hamiltonian within the Hartree-Fock approximation. They have also implemented the modified spin wave theory to calculate the thermodynamic functions as the heat capacity and the magnetic susceptibility. More recently, using numerical Lanczos method, the effect of an uniform transverse magnetic field on the ground state phase diagram of a spin-1/2 AF-F chain with anisotropic ferromagnetic coupling is studied[24]. The Hamiltonian of the model under consideration on a periodic chain of N sites is given by

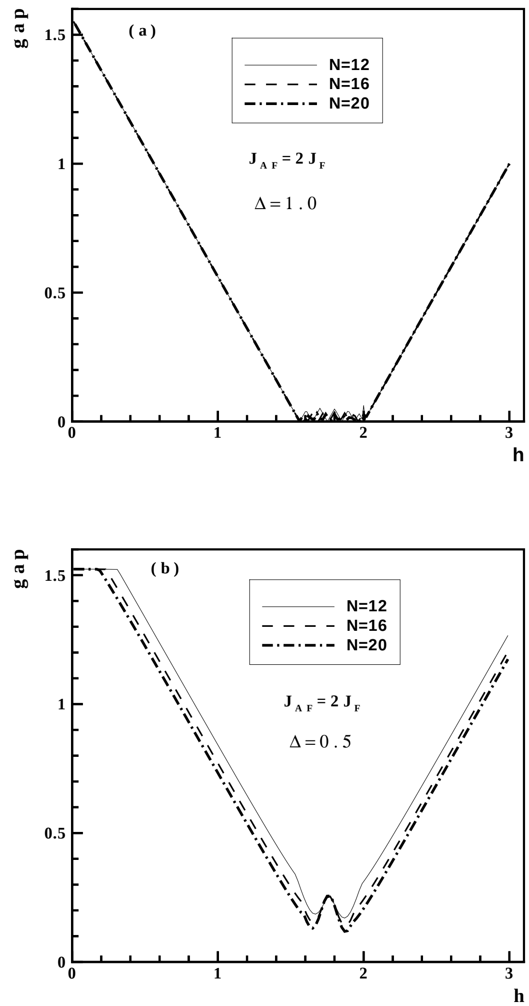

FIG. 2: a. The excitation gap of a spin-1/2 AF-F chain for isotropic case $\Delta = 1.0$ in the uniform magnetic field for different size number ($N = 12, 16, 20$). b. The excitation gap of a spin-1/2 AF-F chain in the uniform transverse magnetic field with anisotropic ferromagnetic coupling $\Delta = 0.5$, for different size number ($N = 12, 16, 20$).

$$
\begin{aligned}
H &= J_{AF}\sum_{j=1}^{N/2}[S^x_{2j-1}S^x_{2j} + S^y_{2j-1}S^y_{2j} + S^z_{2j-1}S^z_{2j}] \\
&- J_F\sum_{j=1}^{N/2}[S^x_{2j}S^x_{2j+1} + S^y_{2j}S^y_{2j+1} + \Delta S^z_{2j}S^z_{2j+1}] \\
&+ h\sum_{j=1}^{N} S^x_j. \qquad (7)
\end{aligned}
$$

Where $S^{x,y,z}_j$ are spin-1/2 operators on the j-th site. J_F and J_{AF} denote the ferromagnetic and antiferromagnetic couplings respectively. The limiting case of

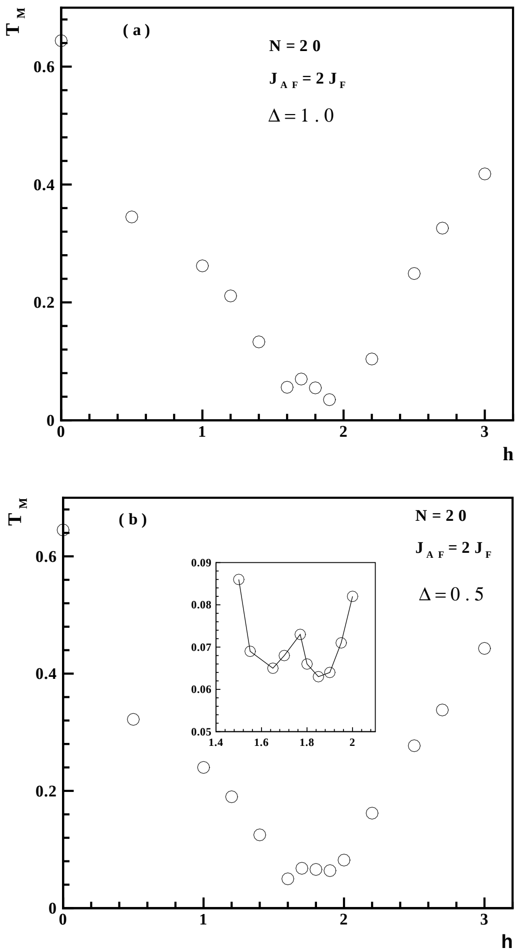

FIG. 3: a. The Schottky heat capacity peak value, T_M, versus the transverse magnetic field, for a spin-1/2 AF-F chain, and isotropic case $\Delta = 1.0$ in the uniform transverse magnetic field for system size: $N = 20$. b. The Schottky heat capacity peak value, T_M, as a function of the magnetic field, for a spin-1/2 AF-F chain in the uniform transverse magnetic field with anisotropic ferromagnetic coupling: $\Delta = 0.5$, and size number: $N = 20$. The inset shows the same quantity in the intermediate magnetic field region, $h_{c_1} < h < h_{c_2}$.

isotropic ferromagnetic coupling corresponds to $\Delta = 1$ and h is the transverse magnetic field. To explore the nature of the excitation spectrum, we use the modified Lanczos method to diagonalize numerically finite chains ($N = 12, 16, 20, 24$). The energies of the few lowest eigenstates were obtained for the chains with periodic boundary conditions. First, we have computed the three lowest energy eigenvalues of $N = 12, 16, 20$ chain with $J_{AF} = 2J_F$ and different values of the anisotropy parameter Δ.

In Fig. 2a we have plotted results of calculations for the isotropic case $\Delta = 1.0$. The excitation gap is determined[24] in the system as the difference between the first excited state and the ground state. As it is clearly seen from this figure in the case of zero magnetic field the spectrum of the model is gapped. For $h \neq 0$ the gap decreases linearly with h and vanishes at the critical field, $h_{c_1} = 1.55 \pm 0.01$. This is the first level crossing between the ground state energy and the first excited state. To get an accurate estimate of h_{c_1} we have obtained the first level crossing for system sizes of $N = 12, 14, ..., 24$. The finite size behavior of these values lead us to $h_{c_1} = 1.55 \pm 0.01$ for $N \longrightarrow \infty$. The spectrum remains gapless for $h_{c_1} < h < h_{c_2}$ and becomes once again gapped for $h > h_{c_2} = 2.0$. With increasing field, for $h > h_{c_2}$ the gap increases linearly with h. In the region $h_{c_1} < h < h_{c_2}$ we also observe numerous additional level crossing between the lowest eigenstates. These level crossing lead to incommensurate effects that manifest themselves in the oscillatory behavior of the spin correlation functions. All crossings disappear at $h > h_{c_2}$ and the correlation functions do not contain oscillatory terms in this region of the phase diagram.

In marked contrast with the isotropic case, the similar analysis of the few lowest levels for an anisotropic AF-F chain in the presence of a transverse magnetic field reveal a principally different behavior. The gap as a function of the transverse magnetic field h has been computed for the anisotropy parameter $\Delta = 0.5$ and different chain lengths $N = 12, 16, 20$. In Fig.2b we have plotted results of these calculations. As it is seen from the figure, the excitation spectrum in this case is gapful except at the two critical fields $h_{c_1} = 1.64 \pm 0.01$ and $h_{c_2} = 1.88 \pm 0.01$[24]. We have employed the phenomenological renormalization group (PRG) method[25] to determine these critical fields (h_{c_1} and h_{c_2}). The PRG equation is

$$(N + 4)gap(N + 4, h') = Ngap(N, h), \tag{8}$$

where $gap(N, h) = E_1(N, h) - E_0(N, h)$ is the energy gap value for chain length N in a magnetic field h. At the critical point, $N(E_1 - E_0)$ should be size independent for large enough systems in which the contribution from irrelevant operators is negligible. Thus, we accurately determined the critical points by the PRG method. We defined $h_c(N, N + 4)$ as the N-dependent fixed point of Eq. 8, and it is extrapolated to the thermodynamic limit in order to estimate h_c. At the critical point $h = h' = h_c$, therefore, the curves of $N(E_1 - E_0)$ vs h for sizes N and $N + 4$ cross at certain values $h_{c_1}(N, N + 4)$ and $h_{c_2}(N, N + 4)$ (finite-size critical points). The thermodynamic critical points (h_{c_1} and h_{c_2}) are obtained by appropriately extrapolating $h_{c_1}(N, N+4)$ or $h_{c_2}(N, N+4)$ to $N \to \infty$.

In the region $h_{c_1} < h < h_{c_2}$ the spin gap, which appears at $h > h_{c_1}$, first increases vs external field and after passing a maximum decreases to vanish at h_{c_2}. At $h > h_{c_2}$ the gap once again opens and, for a sufficiently large transverse field becomes proportional to h. To study the finite-temperature properties of the model, we have used the Jaklič formalism. We have computed a hundred lowest eigenvalues of the energies. We have considered different values of the transverse magnetic field,

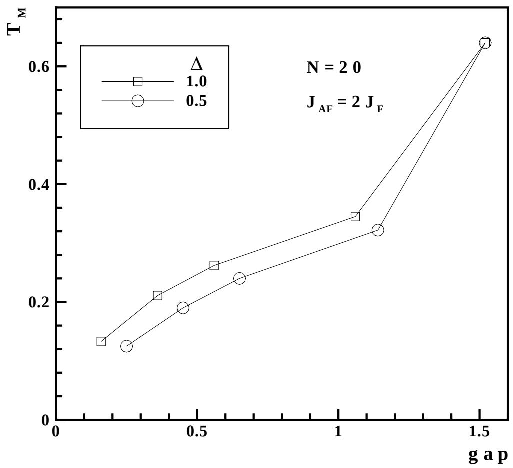

FIG. 4: The Schottky heat capacity peak value, T_M, versus the energy gap for a spin-1/2 AF-F chain with anisotropic ferromagnetic couplings: $\Delta = 1.0$ and $\Delta = 0.5$, and size number: $N = 20$.

h, and anisotropy parameter Δ. Therefore using these hundred eigen-energies, we have computed the heat capacity as a function of the temperature (T). The position of the Schottky heat capacity peak, T_M is determined as T_M. In Fig. 3a we have plotted T_M as a function of the magnetic field h. To arrive at this plot, we have considered $J_{AF} = 2J_F$, $\Delta = 1$ and $N = 20$. As it is clearly seen from this figure, the position of the Schottky heat capacity peak, T_M, T_M, decreases by increasing the magnetic field up to the critical field, h_{c_1}. In the intermediate region of the magnetic filed, $h_{c_1} < h < h_{c_2}$, T_M is independent of magnetic field. The anomaly behavior is the result of the finite size effects. With increasing the magnetic field, for $h > h_{c_2}$, T_M increases almost linearly.

It is surprising which the behavior of T_M versus the magnetic field is in complete agreement with the gap behavior respect to the magnetic filed. Thus we conclude that the energy gap sign on the position of the Schottky heat capacity peak. To confirm our idea, we have plotted T_M vs the transverse magnetic field for $J_{AF} = 2J_F$, the anisotropy parameter $\Delta = 0.5$ and $N = 20$ in Fig. 3b. As we can see from this figure for low transverse magnetic field, $h < h_{c_1}$, the behavior of T_M is the same as the isotropic case. But in the intermediate region, $h_{c_1} < h < h_{c_2}$, T_M first increases vs transverse field and after passing a maximum, decreases up to h_{c_2} (see the inset of the Fig. 3b). For the higher transverse magnetic field, $h > h_{c_2}$, the position of the Schottky heat capacity peak increases as a previous one. This behavior of the T_M is in complete agreement with the effect of the transverse magnetic field on the energy gap (Fig. 2b).

Finally, we have plotted T_M versus the energy gap for $N = 20$, $J_{AF} = 2J_F$ and different values of the anisotropy parameter $\Delta = 0.5, 1.0$. For convenience, the numerical results of the region $h < h_{c_1}$ are showed. It is clearly seen, that the possition of the Schottky heat capacity peak T_M, increases by increasing the energy gap of the system. This is in well agreement with results obtained within the two-level model.

B. The 1D AF-Heisenberg model in a staggered field

The general feature developed for the alternating spin-1/2 chains in a magnetic field can be applied to the 1D Heisenberg Hamiltonian with a staggered magnetic field h_s,

$$H = J\sum_{i=1}^{N}[\overrightarrow{S}_i.\overrightarrow{S}_{i+1} + h_s(-1)^i S_i^z]. \tag{9}$$

It is expected[26,27,28,29] that the staggered field induces an excitation gap in the $S = \frac{1}{2}$ AF-Heisenberg chain, which should be otherwise gapless. The excitation gap caused by the staggered field is indeed found in the real magnets[30,31,32]. In the absence of the staggered field ($h_s = 0$), the eigenspectra is exactly solvable. In the case of the staggered magnetic field ($h_s \neq 0$), the integrability is lost. The staggered magnetic field produces an antiferromagnetic ordered (Neel order) ground-state.

To examine the effect of the staggered magnetic field on the energy gap, we have implemented the modified Lanczos algorithm for finite-size chains $N = 12, 16, 20$ using periodic boundary conditions. The energy gap is determined as the difference between the first excited state and the ground state[14], and calculated for different chain lengths and staggered fields h_s. The energy gap is determined as the difference between the first excited state and the ground state[14].

We have plotted, in Fig. 5a, the energy gap versus the staggered magnetic field h_s. The results have been plotted for different chain sizes $N = 12, 16, 20$. It can be seen, that the spectrum is gapless in the absence of the staggered magnetic field ($h_s = 0$). The application of a staggered magnetic field, induces a gap in the spectrum of the model. With increasing the field, for $h_s > 0$, the energy gap increases with h_s.

Applying the Jakli\v{c} method we have computed a hundred lowest energies for different values of the staggered magnetic field. The heat capacity is computed as a function of the temperature. In Fig. 5b, the position of the Schottky anomaly heat capacity peak, T_M is plotted versus h_s for the chain size $N = 20$. As it is seen from the figure, T_M in this case increases by increasing the staggered magnetic field. This result is in good agreement with the idea that the gap sign on the position of the Schottky heat capacity peak, T_M.

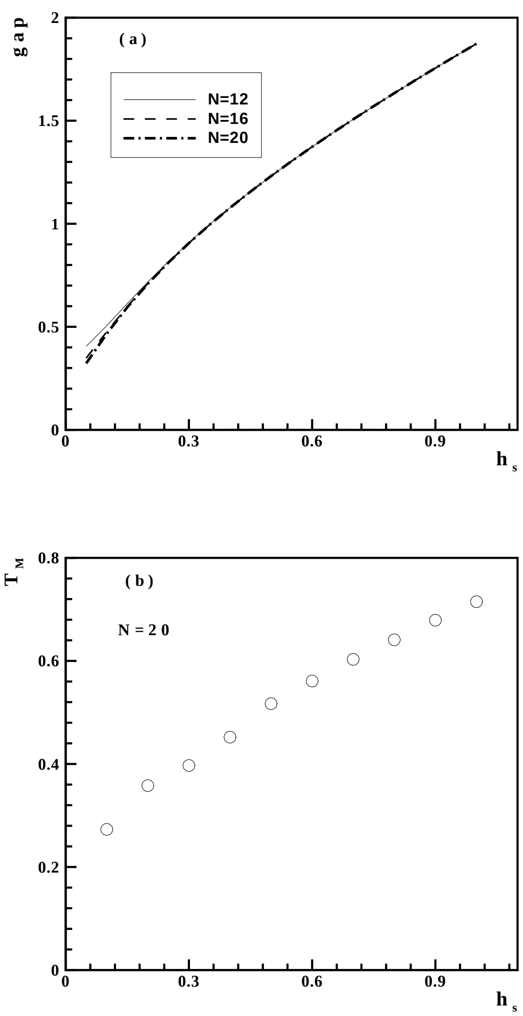

FIG. 5: a. The excitation gap of the 1D AF-Heisenberg model in a staggered field as a function of the magnetic field for different size number ($N = 12, 16, 20$). b. The position of the Schottky heat capacity peak, T_M, for the 1D AF-Heisenberg model in a staggered field versus the staggered magnetic field with size number: $N = 20$.

IV. SUMMARY AND DISCUSSION

Low temperature behavior of the heat capacity of the low-dimensional spin systems is studied using theoretical and numerical approaches. Theoretically, the system is mapped to the well known two-level-system (TLS) model. In this case, the heat capacity is found exactly as a function of the energy gap and the temperature. The position of the Schottky heat capacity peak, T_M, is determined. It is shown that T_M as a function of the control parameter behaves in the same way as the energy gap versus the control parameter. This shows that the gap has an influence on the position of the Schottky heat capacity peak.

Numerically, the finite temperature Lanczos method is applied. The Lanczos method is implemented to obtain a hundred of lowest excited state energies. This formalism is applied to two model chains up to $N = 24$ in length. First, the alternating spin-1/2 chains in a magnetic field are considered. Since, the antiferromagnetic-ferromagnetic (AF-F) chains have a gap in the spin excitation spectrum, they reveal extremely rich quantum behavior in the presence of the magnetic field. The energy gap and heat capacity are computed for both isotropic and anisotropic cases. The numerical results are computed for different values of the external magnetic field. It is shown, in complete agreement with the theoretical results, the field-dependence of the T_M and the energy gap are the same. Finally, the 1D Heisenberg model with a staggered magnetic field h_s is investigated. It is shown that the staggered field induces an excitation gap in the $S = \frac{1}{2}$ AF-Heisenberg chain, which should be otherwise gapless. Using the above numerical procedure, the position of the Schottky heat capacity peak is computed. It is confirm, that the energy gap sign on the Schottky heat capacity peak.

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[1] H. A. Bethe Zphys. **77**, 205 (1931); *ibid*,**150**, 327, (1966).
[2] Kurmann J, Thomas H, and Müller G, Physica **A 112**, 235 (1966); *ibid*,**150**, 327, (1966).
[3] D. V. Dmitriev, V. Ya. Krivnov, and A. A. Ovchinnikov, Phys. Rev. **B 65**, 172409 (2002); D. V. Dmitriev, V. Ya. Krivnov, A. A. Ovchinnikov and A. Langari, JETP, **95**, 538 (2002).
[4] Wei Chen, Kazuo Hida, and B. C. Sanctury, Phys. Rev. B **67**, 104401 (2003).
[5] F. D. M. Haldane, Phys. Rev. Lett. **50**, 1153 (1983).
[6] E. Dogotto and T. M. Rice, Sci. **271**, 618 (1996).
[7] K. P. Schmidt and G. S. Uhrig, Mod. Phys. Lett. b **19**, 1179 (2005).
[8] G. Chaboussant, P. A. Crowell, L. P. Levy, O. Piovesana,

A. Madouri and D. Mailly, Phys. Rev. B **55**, 3046 (1997).
[9] G. Chaboussant, M-H. Julien, Y. Fagot-Revurat, M. Hanson, L. P. Levy, C. Berthier, M. Horvatic and O. Piovesana, Euro. Phys. J. B **6**, 167 (1998).
[10] G. Chaboussant, Y. Fagot-Revurat, M-H. Julien, M. Hanson, C. Berthier, M. Horvatic, L. P. Levy, and O. Piovesana, Phys. Rev. Lett. **80**, 2713 (1998).
[11] D. Arcon, A. Lappas, S. Margadonna, K. Prassides, E. Ribera, J. Veciana, C. Rovira, R. T. Henriques, and M. Almeida, Phys. Rev. B **60**, 4191 (1999).
[12] H. Myaffre, H. Horvatic, C. Berthier, M-H. Julien, P. Söransan, L. P. Levy, and O. Piovesana, Phys. Rev. Lett. **85**, 4795 (2000).
[13] B. C. Watson, V. N. Kotov, N. W. Meisel, D. W. Hall, G. E. Granroth, W. T. Montfrooij, S. E. Nagler, D. A. Jensen, R. Backov, M. A. Petruska, G. E. Fanucci, and D. R. Talham, Phys. Rev. Lett. **86**, 5168 (2001).
[14] S. Mahdavifar, Euro. Phys. J. B **55**, 371, (2007).
[15] S. Mahdavifar, Euro. Phys. J. B **59**, 285, (2007).
[16] S. Mahdavifar, J. Phys: Condens. Matter.19, 406222 (2007).
[17] N. D. Mermin, H. Wagner, Phys. Rev. Lett. **17**, 1133, (1966).
[18] For example see: R. Cubo, Statistical Mechanics, Mir, Moscow, (1967).
[19] For example see: B.Wunderlich, H.Baur, Adv. Polymer Sci.**7**,151 Heat capacity of linear high polymers, (1970)
[20] C. Lanczos, J. Res. Natl. Bur. Stand. **45**, 255, (1950).
[21] J. Jaklič and P. Prelovšec, Phys. Rev. B **7**, 5065, (1994).
[22] T. Sakai: J. Phys. Soc. Jpn. **64**, 251 (1995).
[23] S. Yamamoto et. al,: Fiz. Nizk. Temp. **31**, 974 (2005).
[24] S. Mahdavifar, and A. Akbari, Accepted to J. Phys. Soc. Jpn (2007).
[25] M. N. Barber: *Phase Transitions and Critical Phenomena* , edited by C. Domb and J. L. Lebowitz (Academic Press, New York, 1983) vol. **8**, 146.
[26] M. Oshikawa and I. Affleck, Phys. Rev. Lett. **79**, 2883 (1997); Phys. Rev. B **60**, 1038 (1999).
[27] Y. -J. Wang, F. H. L. Essler, M. Fabrizio and A. A. Nersesyan, Phys. Rev. B **66**, 024412 (2002).
[28] M. Sato and M. Oshikawa, Phys. Rev. B **69**, 054406 (2004)
[29] F. C. Alcaraz and A. L. Malvazzi, J. Phys. A **28**, 1521 (1995).
[30] D. C. Dender, P. R. Hammar, D. H. Reich, C. Broholm and G. Aeppli, Phys. Rev. Lett. **79**, 1750 (1997).
[31] M. Kohgi, K. Iwasa, J. M. Mignot, B. Fak, P. Gegenwart, M. Lang, A. Ochiai, H. Aoki and T. Suzuki, Phys. Rev. Lett. **86**, 2439 (2001).
[32] R. Feyerherm, S. Abens, D. Gunther, T. Ishida, M. Meibner, M. Meschke, N. Nogami and M. Steiner, J. Phys. Condens. Matter **12**, 8495 (2000).